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Spontaneous magnetization of the square 2D Ising lattice with nearest- and weak next-nearest-neighbour interactions

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We show that the square two-dimensional (2D) Ising lattice with nearest- (J) and weak next-nearest-neighbour interactions (J_d) can be mapped on a square 2D Ising lattice that has only nearest neighbour interactions (J^*). For $J_d/J << 1$ the transformation equation has the simple form $J^* = J + \sqrt{2}J_d$. This result can be used to derive expressions for several thermodynamic functions of the square 2D Ising lattice with weak next-nearest-neighbour interactions. As an example we consider the spontaneous magnetization and compare it with low-temperature series expansion results.

Keywords: phase transitions; Ising models; spontaneous magnetization; critical phenomena

1. Introduction

In 1944, Onsager [1] exactly solved the square 2D Ising model with nearest-neighbour interactions in the absence of an external magnetic field. Onsager derived expressions for the free energy per spin and several other thermodynamic functions, such as the energy and the heat capacity. A few years later he also obtained an expression for spontaneous magnetization. He, however, never made the effort to publish this important result. Eventually, it was the China-born American physicist, C.N. Yang, who succeeded in re-deriving Onsager's result [2].

The 2D Ising model that includes, besides nearest-neighbour interactions, also next-nearest-neighbour interactions has not been solved exactly yet. Despite the simplicity of this model, its phase diagram is amazingly rich. It contains ferromagnetic, antiferromagnetic, paramagnetic and superantiferromagnetic phases. Several approaches, such as series expansions [3], finite scaling of the transfer matrix [4,5] and Monte Carlo simulations [6] have been applied in order to find points on the critical lines that separate the different phases of this model from each other.

Here we revisit the square 2D Ising lattice with nearest- and next-nearest-neighbour interactions. The method we apply is referred to as the boundary tension method and relies on finding an expression for the boundary free energy between two phases with different

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spin orientation. The critical temperature is found by setting the boundary free energy equal to zero. Although this method is an approximate method, it turns out be very accurate in the limit of a vanishing next-nearest-neighbour interaction. We show that in this region of the phase diagram the 2D Ising model with nearest- and weak next-nearest-neighbour interactions can be mapped on a 2D Ising model that includes nearest-neighbour interactions only. The mapping procedure allows one to find expressions for a number of thermodynamic functions of the square 2D Ising model with nearest- and weak next-nearest-neighbour interactions, such as the spontaneous magnetisation, the free energy per spin, the heat capacity and the critical temperature.

2. Results and discussion

In the literature, several routes to determine the boundary tension of a number of 2D and 3D lattices without crossing bonds have been put forward [7–10]. Recently, we derived an expression for the boundary tension (or boundary free energy) along the high symmetry (10) direction, $F_{(10)}$, of a square 2D Ising model with crossing bonds [11]. We will briefly repeat the derivation here. For the sake of simplicity we will restrict ourselves here to a simple square 2D lattice with ferromagnetic nearest-neighbour interactions ($J > 0$). The next-nearest-neighbour interaction (J_d) can either be ferromagnetic or antiferromagnetic. We consider a boundary running along the (10) direction that separates two regions with opposite spins. At zero temperature the boundary is kink-less and the formation energy per unit spin is given by, $E_{(10)} = 2J + 4J_d$. With increasing temperature the formation of kinks in the boundary allows the boundary to meander. This meandering increases the entropy and thus lowers the free energy of the boundary. However, the creation of kinks in the boundary costs energy and thus increases the energy of the boundary. The formation energy of a kink with length n (measured in the number of spins) in a (10) boundary is given by $E_{n,(10)} = 2nJ + 4(n-1)J_d$ [12]. The partition function of the (01) boundary per spin is then,

$$Z_{(10)} = \sum_i e^{-E_i/k_BT} = e^{-2(J+2J_d)/k_BT}\left[1 + 2\sum_{n=1}^{\infty} e^{-(2nJ+4(n-1)J_d)/k_BT}\right], \tag{1}$$

where we have summed over all possible configurations of an elementary boundary segment. The boundary free energy per spin can be extracted from the expression, $F_{(10)} = -k_BT \ln[Z_{(10)}]$. We find

$$F_{(10)} = 2J + 4J_d - k_BT \ln\left[1 + \frac{2e^{-2J/k_BT}}{1 - e^{-(2J+4J_d)/k_BT}}\right]. \tag{2}$$

For a vanishing next-nearest-neighbour interaction the original result of Onsager, i.e. $F_{(10)} = 2J - k_BT \ \ln[1 + e^{-2J/k_BT}/1 - e^{-2J/k_BT}]$, is recovered [1]. The ferromagnetic to paramagnetic phase transition occurs at a temperature T_c, which can be found by setting the boundary tension equal to zero [1]. We find,

$$2e^{-2H_{\omega}} + e^{-4H_{\omega}}\left(2 - e^{-4H_{d,c}}\right) = e^{4H_{d,\omega}}, \tag{3}$$

where we have introduced for convenience the parameters $H_{(c)} = J/k_BT_{(c)}$ and $H_{d,(c)} = J_d/k_BT_{(c)}$. This approximation gives an accurate estimate for the transition temperature, even for relatively large values of H_d/H. For instance, at $H_d/H = 1/4$ the critical temperature deviates less than 1% from the most accurate available numerical data obtained by Monte Carlo simulations [6], series expansions [3] and finite-size scaling of transfer matrix results [5].

The well-known Onsager relation for the ferromagnetic to paramagnetic phase transition, i.e. $\sinh(2H_c) = 1$, is recaptured for $H_d = 0$. The critical line of the phase diagram that separates the paramagnetic phase from the ferromagnetic phase is in good agreement with numerically available data, such as series expansions [3], finite scaling of the transfer matrix [4,5] and Monte Carlo results [6]. However, the critical line does not reproduce the predicted cusp behaviour for vanishing nearest-neighbour coupling [13]. In contrast, in the limit of small next-nearest-neighbour interactions the results are remarkably accurate. The slope of the critical line in the Onsager point, as extracted from Equation (3), i.e. $(\partial H_d/\partial H)H_c$, is given by $-1/2\sqrt{2}$. This result turns out to be exact and has first been derived by Burkhardt [14] using universality arguments. This slope results in a shift in the critical temperature of $\sqrt{2}H_d/H$ with respect to the Onsager point (T_{c0}) when comparing the zero and non-zero next-nearest-neighbour square 2D Ising models with each other. The latter result is in good agreement with series expansion by Dalton and Wood [15]. These authors derived power series expansions for the partition function near the critical point. Using this approach they found a shift in the critical temperature of 1.45 H_d/H. However, these results deviate somewhat from the result obtained by Herman and Dorfman [16] using a thermodynamic perturbation theory. These authors found a shift in the critical temperature that is in first order given by 0.90 H_d/H.

Since the boundary tension expression is very accurate for small next-nearest-neighbour interactions, i.e. $|H_d| << H$, we will restrict ourselves to this regime [17]. Using some mathematics it can be shown that for small H_d Equation (3) can be written in the elegant Onsager form,

$$2e^{-2H_c^*} + e^{-4H_c^*} = 1 \quad \text{or} \quad \sinh\left(2H_c^*\right) = 1 \tag{4a}$$

with

$$H^* = H + \sqrt{2}H_d. \tag{4b}$$

This result implies that for small next-nearest-neighbour interactions, the square 2D Ising lattice with nearest- and next-nearest-neighbour interactions can be mapped on a square 2D Ising lattice with nearest-neighbour interactions only. The mapping equation has the particularly elegant form $H^* = H + \sqrt{2}H_d$. Hence, we can simply replace H in the exact thermodynamic functions of the isotropic square 2D Ising model with nearest-neighbour interactions by $H + \sqrt{2}H_d$. As an illustrative example we consider the spontaneous magnetisation, $M(T)$. By inserting $H + \sqrt{2}H_d$ in Yang's expression [2] for the spontaneous magnetisation expression we find,

$$M(T) = \left(1 - \sinh^{-4}\left(2\left(H + \sqrt{2}H_d\right)\right)\right)^{1/8}. \tag{5}$$

This fact that the result does not deviate much from Yang's expression [2] is not surprising, since it is generally accepted that the square 2D Ising lattices with and without next-nearest-neighbour interactions fall in the same universality class (at least for weak next-nearest-neighbour coupling [18]).

In order to check the validity of our results we compare our expression of the spontaneous magnetization with low-temperature series expansions of the spontaneous magnetization [19]. Lee and Lin [19] calculated the low-temperature series expansion of the spontaneous magnetization for the square 2D Ising lattice with nearest and next-nearest-neighbour interactions up to the twenty-fourth order. We adopt the notation of Lee and Lin and write,

$$x = e^{-4J/k_BT} \text{ and } y = e^{-4J_d/k_BT} \tag{6a}$$

The spontaneous magnetization, $M(T)$, is given by [19]

$$M(T) = 1 - 2x^2y^2 + \sum_{i=7}^{\infty} M_i \tag{6b}$$

where

$$\begin{aligned}
M_7 &= -8x^3y^4 - 8x^4y^3 \\
M_8 &= 18x^4y^4 \\
M_9 &= -24x^4y^5 \\
M_{10} &= -20x^4y^6 - 48x^5y^5 - 36x^6y^4 \\
M_{11} &= 80x^5y^6 + 168x^6y^5 \\
M_{12} &= -144x^5y^7 - 364x^6y^6 - 8x^8y^4 \\
M_{13} &= -40x^5y^8 + 144x^6y^7 - 288x^7y^6 - 144x^8y^5 \\
M_{14} &= -52x^6y^8 + 1184x^7y^7 + 1160x^8y^6 \\
M_{15} &= -504x^6y^9 - 2704x^7y^8 - 3872x^8y^7 - 40x^9y^6 - 80x^{10}y^5 \\
M_{16} &= -70x^6y^{10} + 1440x^7y^9 + 5358x^8y^8 - 1712x^9y^7 - 340x^{10}y^6 \\
M_{17} &= -1648x^7y^{10} - 2704x^8y^9 + 11464x^9y^8 + 6632x^{10}y^7 - 24x^{12}y^5 \\
M_{18} &= -1344x^7y^{11} - 8064x^8y^{10} - 37328x^9y^9 \\
&\quad - 33356x^{10}y^8 - 576x^{11}y^7 - 480x^{12}y^6 \\
M_{19} &= -112x^7y^{12} + 2672x^8y^{11} + 56368x^9y^{10} \\
&\quad + 76880x^{10}y^9 - 7664x^{11}y^8 + 816x^{12}y^7 \\
M_{20} &= -8524x^8y^{12} - 57136x^9y^{11} - 84864x^{10}y^{10} \\
&\quad + 88608x^{11}y^9 + 29968x^{12}y^8 - 112x^{13}y^7 - 308x^{14}y^6 \\
M_{21} &= -3024x^8y^{13} - 10696x^9y^{12} - 45648x^{10}y^{11} \\
&\quad - 407200x^{11}y^{10} - 239176x^{12}y^9 - 5584x^{13}y^8 - 1568x^{14}y^7 \\
M_{22} &= -168x^8y^{14} - 13168x^9y^{13} + 167404x^{10}y^{12} \\
&\quad + 963264x^{11}y^{11} + 828616x^{12}y^{10} - 16384x^{13}y^9 \\
&\quad + 16156x^{14}y^8 - 96x^{16}y^6 \\
M_{23} &= -29752x^9y^{14} - 302640x^{10}y^{13} - 1460808x^{11}y^{12} \\
&\quad - 1457144x^{12}y^{11} + 552688x^{13}y^{10} + 87168x^{14}y^9 \\
&\quad + 2744x^{15}y^8 + 10576x^{16}y^7 \\
M_{24} &= -5856x^9y^{15} - 35016x^{10}y^{14} + 783760x^{11}y^{13} \\
&\quad + 262764x^{12}y^{12} - 4047776x^{13}y^{11} - 1612450x^{14}y^{10} \\
&\quad - 34624x^{15}y^9 + 2136x^{16}y^8 - 18x^{18}y^6
\end{aligned} \tag{6c}$$

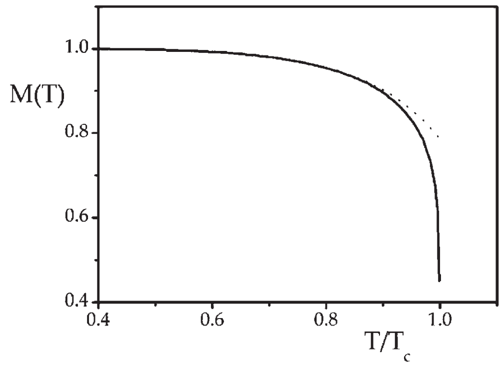

Figure 1. Spontaneous magnetization of the square 2D Ising by Yang [2] (solid line) and low-temperature series expansion results by Lee and Lin [19] (dotted line) vs. temperature for $J_d/J=0$. The deviation between both curves is <0.001 for temperatures lower than $T/T_c=0.8$.

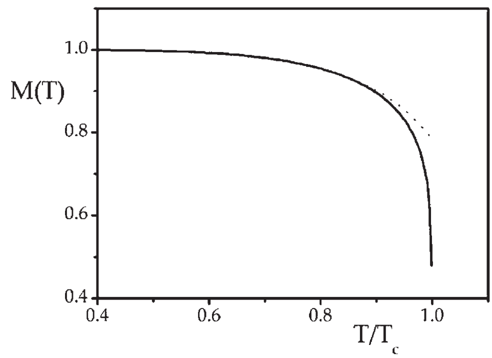

Figure 2. Spontaneous magnetization as obtained by Equation (5) (solid line) and low-temperature series expansion results by Lee and Lin [19] (dotted line) vs. temperature for $J_d/J=0.01$. The deviation between both curves is <0.001 for temperatures lower than $T/T_c=0.8$.

In Figure 1, we have plotted the exact solution of the spontaneous magnetisation of the square 2D Ising lattice with nearest-neighbour interaction [2] and the series expansion results of Lee and Lin [19] for $J_d=0$. For temperatures lower than $T/T_c=0.8$ the deviation is <0.001, however near T_c the series expansion results deviate substantially from the exact solution. In Figure 2, we have plotted the spontaneous magnetization as obtained by Equation (5) and series expansion results *versus* temperature for $J_d/J=0.01$. For temperatures lower than $T/T_c=0.8$, we again find a deviation that is comparable to, i.e. smaller than 0.001, the deviation found in Figure 1. Even for $J_d/J=0.1$, the difference between Equation (5) and the series expansion results is only 0.0027 at $T/T_c=0.8$. On the basis of these findings we conclude that our approximation of the spontaneous magnetisation is very accurate for small values of J_d/J. In addition, in contrast to the series expansion result, our expression nicely vanishes at T_c with the correct critical exponent 1/8.

3. Conclusions

We have shown that the square 2D Ising lattice with nearest-neighbour ($H=J/k_BT$) and weak next-nearest-neighbour ($H_d/H << 1$) interactions can be mapped on the square 2D

Ising lattice with nearest-neighbour ($H^* = J^*/k_B T$) interactions only via the transformation: $H^* = H + \sqrt{2}H_d$. This result leads to valuable expressions for a number of thermodynamic functions.

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